Investigation of continuous-time quantum walk on root lattice A_n and honeycomb lattice

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Abstract

The continuous-time quantum walk (CTQW) on root lattice A_n (known as hexagonal lattice for $n = 2$) and honeycomb one is investigated by using spectral distribution method. To this aim, some association schemes are constructed from abelian group $Z_m^{\otimes n}$ and two copies of finite hexagonal lattices, such that their underlying graphs tend to root lattice A_n and honeycomb one, as the size of the underlying graphs grows to infinity. The CTQW on these underlying graphs is investigated by using the spectral distribution method and stratification of the graphs based on Terwilliger algebra, where we get the required results for root lattice A_n and honeycomb one, from large enough underlying graphs. Moreover, by using the stationary phase method, the long time behavior of CTQW on infinite graphs is approximated with finite ones. Also it is shown that the Bose-Mesner algebras of our constructed association schemes (called n-variable P-polynomial) can be generated by n commuting generators, where raising, flat and lowering operators (as elements of Terwilliger algebra) are associated with each generator. A system of n-variable orthogonal polynomials which are special cases of *generalized* Gegenbauer polynomials is constructed, where the probability amplitudes are given by integrals over these polynomials or their linear combinations. Finally the suppersymmetric structure of finite honeycomb lattices is revealed.

Keywords: underlying graphs of association schemes, continuous-time quantum walk, orthogonal polynomials , spectral distribution.

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1 Introduction

Quantum walks have recently been introduced and investigated with the hope that they may be useful in constructing new efficient quantum algorithms (for reviews of quantum walks, see [1], [2], [3]). A study of random walks on simple lattices is well known in physics(see [4]). Recent studies of quantum walks on more general graphs were described in [5], [6], [1], [7], [8]. Some of these works study the problem in the important context of algorithmic problems on graphs and suggest that quantum walks is a promising algorithmic technique for designing future quantum algorithms.

On the other hand, the theory of association schemes [9] (the term of association scheme was first coined by R. C. Bose and T. Shimamoto in [10]) has its origin in the design of statistical experiments. The connection of association schemes to algebraic codes, strongly regular graphs, distance regular graphs, design theory etc., further intensified their study. A further step in the study of association schemes was their algebraization. This formulation was done by R. C. Bose and D. M. Mesner who introduced an algebra generated by the adjacency matrices of the association scheme, known as Bose-Mesner algebra. The other formulation was done by P. Terwilliger, known as the Terwilliger algebra. This algebra has been used to study P- and Q-polynomial schemes [11], group schemes [12, 13], and Doob schemes [14].

Authors in [15, 16, 17] have introduced a new method for calculating the probability amplitudes of CTQW on particular graphs based on spectral distribution and algebraic combinatorics structures of the graphs, where a canonical relation between the interacting Fock space of CTQW (i.e., Hilbert space of CTQW starting from a given site which consists of irreducible submodule of Terwilliger algebra with maximal dimension) and a system of orthogonal polynomials has been established which leads to the notion of quantum decomposition (QD) introduced in [18, 19]. In [15, 16, 19], only the particular graphs of QD type have been studied, where the adjacency matrices posses quantum decomposition and one can give the graph a

three-term recursion structure. Then, by employing the three-term recursion structure of the graph, one can define the Stieltjes transform of spectral distribution and obtain the corresponding spectral distribution via inverse Stieltjes transform. The QD property is inherent in underlying graphs of P-polynomial association schemes (for more details of P-polynomial association schemes, see [20], [21], [22], [11], [23]) due to the algebraic combinatorics structure of schemes, particularly the existence of raising, flat and lowering operators.

Here in this work, we investigate CTQW on root lattice A_n and honeycomb one by using spectral distribution method. In particular, we discuss the root lattice A_2 (called hexagonal or triangular lattice) in more details, and then generalize the results to the case of A_n. To this purpose, first we construct some interesting association schemes from abelian group $Z_m^{\otimes n}$ and finite honeycomb lattice, where in the first case, the orbits of Weyl group corresponding to the finite lattice, define a translation invariant (non-symmetric) association scheme on $Z_m^{\otimes n}$. Then, by symmetrization method, we construct a new symmetric association scheme, where CTQW is investigated on its underlying graph. In the latter case , we construct the association scheme from two copies of finite hexagonal lattices, where the corresponding adjacency matrix A is defined suitably from the adjacency matrix of finite hexagonal lattice and the other adjacency matrices are constructed via powers of A (in this case we have not a systematic procedure for construction of association scheme as in the first case). These association schemes have the privileges that, for large enough size of their underlying graphs, they tend to root lattice A_n and honeycomb one, respectively. By using spectral distribution method, we study CTQW on these underlying graphs via their algebraic combinatorics structures such as (reference state dependent) Terwilliger algebras. By choosing the starting site of the walk as reference state, the Terwilliger algebra connected with this choice, stratifies the graph into disjoint unions of strata, where the amplitudes of observing the CTQW on all sites belonging to a given stratum are the same. This stratification is different from the one based on distance, i.e., it is possible that two strata with the same distance from starting site posses different probability

amplitudes. Then we study the CTQW on root lattice A_n and honeycomb one by using the results of finite lattices. Moreover, by using the stationary phase method [24], the long time behavior of the quantum walk on infinite graphs is approximated with finite ones. In fact, the numerical results show that, the A_2 (honeycomb) lattice can be approximated by a finite hexagonal (finite honeycomb) lattice for m larger than ~ 50 (~ 60) and times $t \sim 1000$ ($t \sim 700$).

Another interesting property of constructed association schemes from $Z_m^{\otimes n}$ is that, their corresponding Bose-Mesner algebras are generated by n commuting generators. In particular, the adjacency matrices are n-variable polynomials of the generators, where recursion relations for the polynomials are given by using the structure of the association schemes. This property allows us to generalize the notion of P-polynomial association schemes to *n-variable* P-polynomial association schemes, where the spectral distributions associated with the generators are functions of n variables (variables assigned to the generators). Also, we associate raising, lowering and flat operators with each generator via the elements of corresponding Terwilliger algebra. Then, by using the recursion relations associated with the Bose-Mesner algebra, we construct a system of n-variable orthogonal polynomials which are special cases of orthogonal polynomials known as *generalized* Gegenbauer polynomials [25], [26], where the probability amplitudes of the walk are given by integrals over these polynomials or their linear combinations. In fact, it is shown that similar to the P-polynomial case, there is a canonical isomorphism from the interacting Fock space of CTQW on finite root lattice A_n onto the closed linear span of these orthogonal polynomials. Finally, we reveal the suppersymmetric structure of finite honeycomb lattices in the appendix.

The organization of the paper is as follows. In section 2, we introduce briefly root lattice A_n and honeycomb lattice. In section 3, we give a brief outline of association schemes, Bose-Mesner and Terwilliger algebras. In section 4, we give an algorithm for constructing some underlying graphs of so called two-variable P-polynomial association schemes and then

following ref.[16], we stratify the underlying graphs of constructed two-variable P-polynomial association schemes. In section 5, we give a brief review of spectral distribution method and discuss the construction of two-variable orthogonal polynomials. Section 6, is devoted to CTQW on hexagonal lattice and honeycomb one, by using spectral distribution method. Also, the asymptotic behavior of probability amplitudes of the walk at large time t, is discussed. Finally, we generalize the discussions of A_2 to A_n in section 7. The paper is ended with a brief conclusion together with an appendix on the suppersymmetric structure of finite honeycomb lattices.

2 Root lattice A_n and honeycomb lattice

2.1 Root lattice A_n

It is well known that a Coxeter-Dynkin diagram determines a system of simple roots in the Euclidean space E_n. The finite group W, generated by the reflections through the hyperplanes perpendicular to roots α_i, $i = 1, ..., n$

$$r_i(\beta) = \beta - 2\frac{(\alpha_i, \beta)}{(\alpha_i, \alpha_i)}\alpha_i \in R, \tag{2-1}$$

is called a Weyl group (for the theory of such groups, see [27] and [28]). An action of elements of the Wyle group W upon simple roots leads to a finite system of vectors, which is invariant with respect to W. A set of all these vectors is called a system of roots associated with a given Coxeter-Dynkin diagram (for a description of the correspondence between simple Lie algebras and Coxeter-Dynkin diagrams, see, for example, [29]). It is proven that roots of R are linear combinations of simple roots with integral coefficients. Moreover, there exist no roots which are linear combinations of simple roots α_i, $i = 1, 2, ..., n$, both with positive and negative coefficients. The set of all linear combinations

$$Q = \{\sum_{i=1}^{n} a_i\alpha_i \ \mid \ a_i \in Z\} \equiv \bigoplus_i Z\alpha_i, \tag{2-2}$$

is called a root lattice corresponding to a given Coxeter-Dynkin diagram. Root system R which corresponds to Coxeter-Dynkin diagram of Lie algebra of the group $SU(n+1)$, gives root lattice A_n. For example root system A_2 (corresponding to lie algebra of SU(3)) is shown in Fig.1, where the roots form a regular hexagon and α and β are simple roots (see Fig.1). This lattice sometimes is called hexagonal lattice or triangular lattice.

It is convenient to describe root lattice, Weyl group and its orbits for the case of A_n in the subspace of the Euclidean space E_{n+1} , given by the equation

$$x_1 + x_2 + ... + x_{n+1} = 0, \tag{2-3}$$

where x_1, x_2,..., x_{n+1} are the orthogonal coordinates of a point $x \in E_{n+1}$. The unit vectors in directions of these coordinates are denoted by e_j, respectively. Clearly, $e_i \perp e_j$, $i \neq j$. The set of roots is given by the vectors

$$\alpha_{ij} = e_i - e_j, \quad i \neq j. \tag{2-4}$$

The roots α_{ij}, with $i < j$ are positive and the roots

$$\alpha_i \equiv \alpha_{i,i+1} = e_i - e_{i+1}, \quad i = 1, ..., n, \tag{2-5}$$

constitute the system of simple roots.

By means of the formula (2-1), one can find that the reflection $r_{\alpha_{ij}}$ acts upon the vector $\lambda = \sum_{i=1}^{n+1} m_i e_i$, given by orthogonal coordinates, by permuting the coordinates m_i and m_j. Thus, $W(A_n)$ (Weyl group corresponding to A_n) consists of all permutations of the orthogonal coordinates m_1, m_2,..., m_{n+1} of a point λ, that is, $W(A_n)$ coincides with the symmetric group S_{n+1}. The orbit $O(\lambda)$, $\lambda = (m_1, m_2, ..., m_{n+1})$, consists of all different points $(m_{i_1}, m_{i_2}, ..., m_{i_{n+1}})$ obtained from $(m_1, m_2, ..., m_{n+1})$ by permutations.

For our purposes in this paper, we will construct an underlying graph of association scheme from abelian group $Z_m^{\otimes n}$ $(m \geq 3)$, such that the constructed graph can be viewed as root lattice A_n where Z is replaced with Z_m.

2.2 Honeycomb lattice

The honeycomb lattice is defined by two sets of direction vectors (vectors with integer components), but first we should introduce the notion of odd and even vertices. A vertex is odd if the sum of its components is odd, otherwise it is even. The honeycomb lattice is a two dimensional lattice defined as follows

Definition 4 For an even vertex, the set of direction vectors is $\{(1,0),(-1,0),(0,1)\}$ and for an odd vertex, the set of direction vectors is $\{(1,0),(-1,0),(0,-1)\}$.

A honeycomb structure is related to a hexagonal lattice in the following two ways

(1) The centers of the hexagons of a honeycomb form a hexagonal lattice, with the rows oriented the same.

(2) The vertices of a honeycomb, together with their centers, form a hexagonal lattice, rotated by the angle of $\pi/6$, and scaled by a factor $1/\sqrt{3}$, relative to the other lattice.

The ratio of the number of vertices and the number of hexagons is 2 (see Fig.2).

In section 4, we will construct an underlying graph of association scheme from two copies of hexagonal lattices, where the graph is equivalent to honeycomb lattice as the size of the graph grows to infinity.

3 Association schemes and their Terwilliger algebra

In this section, we give a brief review of some of the main features of symmetric association schemes. For further information about association schemes, the reader is referred to [9], [10], [11].

Definition 3 (Symmetric association schemes). Let V be a set of vertices, and R_i $(i = 0, ..., d)$ be nonempty relations on V. If the following conditions (1), (2), (3), and (4) be satisfied, then the pair $Y = (V, \{R_i\}_{0\leq i\leq d})$ consisting of a vertex set V and a set of relations $\{R_i\}_{0\leq i\leq d}$ is called an association scheme.

(1) $\{R_i\}_{0\leq i\leq d}$ is a partition of $V\times V$

(2) $R_0=\{(\alpha,\alpha):\alpha\in V\}$

(3) $R_i=R_i^t$ for $0\leq i\leq d$, where $R_i^t=\{(\beta,\alpha):(\alpha,\beta)\in R_i\}$

(4) Given $(\alpha,\beta)\in R_k$, $p_{ij}^k=\mid\{\gamma\in V:(\alpha,\beta)\in R_i\ \ and\ \ (\gamma,\beta)\in R_j\}\mid$, where the constants p_{ij}^k are called the intersection numbers, depend only on i,j and k and not on the choice of $(\alpha,\beta)\in R_k$.

The underlying graph $\Gamma=(V,R_1)$ of an association scheme is an undirected connected graph, where the set V and R_1 consist of its vertices and edges, respectively. Obviously replacing R_1 with one of the other relations such as R_i, for $i\neq 0,1$ will also give us an underlying graph $\Gamma=(V,R_i)$ (not necessarily a connected graph) with the same set of vertices but a new set of edges R_i.

Let C denote the field of complex numbers. By $Mat_V(C)$ we mean the set of all $n\times n$ matrices over C whose rows and columns are indexed by V. For each integer i $(0\leq i\leq d)$, let A_i denote the matrix in $Mat_V(C)$ with (α,β)-entry as

$$(A_i)_{\alpha,\beta} \;=\; \begin{cases} 1 & \text{if}\ \ (\alpha,\beta)\in R_i, \\ 0 & \text{otherwise} \end{cases} \qquad\qquad (\alpha,\beta\in V). \tag{3-6}$$

The matrix A_i is called an adjacency matrix of the association scheme. We then have $A_0=I$ (by (2) above) and

$$A_iA_j=\sum_{k=0}^{d}p_{ij}^kA_k, \tag{3-7}$$

so $A_0,A_1,...,A_d$ form a basis for a commutative algebra A of $Mat_V(C)$, where A is known as the Bose-Mesner algebra of Y. Since the matrices A_i commute, they can be diagonalized simultaneously.

We now recall the dual Bose-Mesner algebra of Y. Given a base vertex $\alpha\in V$, for all integers i define $E^*=E^*(\alpha)\in Mat_V(C)$ $(0\leq i\leq d)$ to be the diagonal matrix with (β,β)-entry

$$(E_i^*)_{\beta,\beta} \;=\; \begin{cases} 1 & \text{if}\ \ (\alpha,\beta)\in R_i, \\ 0 & \text{otherwise} \end{cases} \qquad\qquad (\alpha\in V). \tag{3-8}$$

The matrix E_i^* is called the i-th dual idempotent of Y with respect to α. We shall always set $E_i^* = 0$ for $i < 0$ or $i > d$. From the definition, the dual idempotents satisfy the relations

$$\sum_{i=0}^{d} E_i^* = I, \quad E_i^* E_j^* = \delta_{ij} E_i^* \qquad 0 \leq i, j \leq d. \tag{3-9}$$

It follows that the matrices E_0^*, E_1^*, ..., E_d^* form a basis for a subalgebra $\mathsf{A}^* = \mathsf{A}^*(\alpha)$ of $Mat_V(c)$. A^* is known as the dual Bose-Mesner algebra of Y with respect to α.

Definition 4 (Terwilliger algebra) Let the scheme $Y = (V, \{R_i\}_{0 \leq i \leq d})$ be as in definition 1, pick any $\upsilon \in V$, and let $\mathsf{T} = \mathsf{T}(\upsilon)$ denote the subalgebra of $Mat_V(C)$ generated by the Bose-Mesner algebra A and the dual Bose-Mesner algebra A^*. The algebra T is called Terwilliger algebra of Y with respect to υ.

Let $W = C^V$ denote the vector space over C consisting of column vectors whose coordinates are indexed by V and whose entries are in C. We endow W with the Hermitian inner product $\langle , \rangle$ which satisfies $\langle u, v \rangle = u^t \bar{v}$ for all $u, v \in W$, where t denotes the transpose and - denotes the complex conjugation. For all $\beta \in V$, let $|\beta\rangle$ denote the element of W with a 1 in the β coordinate and 0 in all other coordinates. We observe $\{|\beta\rangle : \beta \in V\}$ is an orthonormal basis for W. Using (3-8) we have

$$W_i = E_i^* W = span\{|\beta\rangle : \beta \in V, (\alpha, \beta) \in R_i\}, \quad 0 \leq i \leq d. \tag{3-10}$$

Now using the relations (3-9), one can show that the operator E_i^* projects W onto W_i, thus we have

$$W = W_0 \oplus W_1 \oplus \cdots \oplus W_d. \tag{3-11}$$

In [16], CTQW on some special kinds of underlying graphs of P-polynomial association schemes has been investigated. It is shown in [20] that in the case of P-polynomial association schemes, $A_i = p_i(A)(0 \leq i \leq d)$, where p_i is a polynomial of degree i with real coefficients. In particular, A generates the Bose-Mesner algebra. Moreover, for a P-polynomial scheme, there is a quantum decomposition for adjacency matrix of the underlying graph, where in

[16], this property has been employed for investigation of CTQW via spectral distribution associated with adjacency matrix. In fact, for P-polynomial schemes a quantum decomposition for adjacency matrix can be defined by the following lemma

Lemma (Terwilliger [11]). Let Γ denote an underlying graph of a P-polynomial association scheme with diameter d. Fix any vertex α of Γ, and write $E_i^* = E_i^*(\alpha)$ $(0 \leq i \leq d)$, $A_1 = A$ and $T = T(\alpha)$. Define $A^- = A^-(\alpha)$, $A^0 = A^0(\alpha)$, $A^+ = A^+(\alpha)$ by

$$A^- = \sum_{i=1}^{d} E_{i-1}^* A E_i^*, \qquad A^0 = \sum_{i=1}^{d} E_i^* A E_i^*, \qquad A^+ = \sum_{i=1}^{d} E_{i+1}^* A E_i^*. \tag{3-12}$$

Then

$$A = A^+ + A^- + A^0, \tag{3-13}$$

where, this is quantum decomposition of adjacency matrix A such that,

$$(A^-)^t = A^+, \qquad (A^0)^t = A^0, \tag{3-14}$$

which can be verified easily.

Note that the above lemma is true only in the cases of P-polynomial association schemes. In this paper we will construct some underlying graphs of association schemes for which the corresponding Bose-Mesner algebras are generated by n commuting operators. Hereafter, we will refer to these types of association schemes as n-variable P-polynomial association schemes. As a generalization of the above lemma to n-variable P-polynomial association schemes, one can define raising, lowering and flat operators as in (3-12) with respect to each generator of Bose-Mesner algebra. In particular, for association scheme derived from $Z_m \times Z_m$, the corresponding Bose-Mesner algebra is generated by two commuting operators A_z and $A_{\bar{z}}$ ($A_{\bar{z}} = A_z^t$), i.e., $A_{kl} = p_{kl}(A_z, A_{\bar{z}})$, where p_{kl} is a polynomial of degree $k+l$ with real coefficients. The raising, lowering and flat operators are defined as in (3-12) with respect to each generator of Bose-Mesner algebra. Explicitly we have

$$A_z^+ := \sum_i E_{i+1}^* A_z E_i^* \qquad A_{\bar{z}}^+ := \sum_i E_{i+1}^* A_{\bar{z}} E_i^*,$$

$$A_{\bar{z}}^{-} := (A_z^{+})^t \qquad A_z^{-} := (A_{\bar{z}}^{+})^t \quad \text{and}$$

$$A_z^0 := \sum_i E_i^* A_z E_i^* \qquad A_{\bar{z}}^0 := \sum_i E_i^* A_{\bar{z}} E_i^*. \tag{3-15}$$

Similar to P-polynomial association schemes, we have

$$A_z = A_z^+ + A_z^- + A_z^0, \quad A_{\bar{z}} = A_{\bar{z}}^+ + A_{\bar{z}}^- + A_{\bar{z}}^0. \tag{3-16}$$

4 construction of some translation invariant association schemes

In this section, we construct two types of finite underlying graphs of association schemes from finite abelian group $Z_m \times Z_m$ ($m \geq 3$) and two copies of finite hexagonal lattices, such that in the limit of the large size of the graphs, the underlying graphs tend to infinite graphs on root lattice A_2 and honeycomb one, respectively. We will show that the corresponding Bose-Mesner algebras are generated by two commuting operators, in particular all elements of Bose-Mesner algebras are two-variable polynomials of the generators. We will refer to these schemes as two-variable P-polynomial association schemes. To our purpose, first we give some definitions.

Definition 6 Let A be a finite multiplicative abelian group and $R = \{R_0, ..., R_r\}$ a collection of $r+1$ distinct relations on A forming a partition of the cartesian power A^2. If $(x, y) \in R_i$ implies $(ax, ay) \in R_i$ for all $a \in A$ and $i = 0, 1, ..., r$, then P is called translation invariant.

Definition 7 A partition $P = \{P_0, ..., P_r\}$ of an abelian group A is called a blueprint [9] if

(1) $P_0 = \{e\}$ (e is the identity of the group),

(2) for $i = 1, ..., r$, if $x \in P_i$ then $x^{-1} \in P_i$ (i.e., $P_i = P_i^{-1}$),

(3) there are integers q_{ij}^k such that if $y \in P_k$ then there are precisely q_{ij}^k elements $x \in P_i$ such that $x^{-1}y \in P_j$.

Now let A be an abelian group, and $P = \{P_0, ..., P_r\}$ be a blueprint of A. Let $\Gamma(P) =$

$\{R_0, ..., R_r\}$ be the set of relations

$$R_i = \{(x, y) \in A^2 \ | \ x^{-1}y \in P_i\}, \tag{4-17}$$

on A. One can notice that, if P_i is a generating set for the group A, then the underlying graph $\Gamma = (A, R_i)$ is called a Cayley graph on A. From (4-17), it can be easily seen that $R = \{R_0, ..., R_r\}$ forms a translation invariant partition of A^2, where R_0 is diagonal relation. Also from condition (2) in definition 7, $(x, y) \in R_i$ implies that $(y, x) \in R_i$, i.e., $R_i^{-1} = R_i$.

4.1 construction of two-variable P-polynomial association schemes from $Z_m \times Z_m$ $(m \geq 3)$

First we choose the ordering of elements of $Z_m \times Z_m$ as follows

$$V = \{e, a, ..., a^{m-1}, b, ab, ..., a^{m-1}b, ..., b^{m-1}, ab^{m-1}, ..., a^{m-1}b^{m-1}\}, \tag{4-18}$$

where $a^m = b^m = e$. We use the notation (k, l) for the element $a^k b^l$ of the group. Clearly, $(k, l)(k', l') = (k + k', l + l')$ and $(k, l)^{-1} = (-k, -l)$. Then the vertex set V of the graph will be $\{(k, l) : k, l \in \{0, 1, ..., m - 1\}\}$. Now we choose generating set

$$P_{10} = \{(1, 0), (0, 1), (m - 1, m - 1)\}, \tag{4-19}$$

for $Z_m \times Z_m$. With this choice, we obtain Cayley graph $\Gamma = (V, R_{10})$, where $V = Z_m \times Z_m$ and R_{10} is defined by (4-17). Now, we obtain the orbits of Weyl group S_3 (all possible permutations of $(1, 0)$, $(0, 1)$ and $(m - 1, m - 1)$). Then, the orbits

$$P_{kl} := O((k, -l)), \tag{4-20}$$

form a partition P for $Z_m \times Z_m$, where $P_{00} = \{(0, 0)\}$ (in this case, P is called homogeneous). Therefore, by using (4-17), we obtain a coloring for the Cayley graph (V, R_{10}) (with $R_{10} \neq R_{10}^{-1}$). Clearly, for the relations R_{kl} defined by (4-17) we have, $\pi R_{kl} \pi^{-1} = R_{kl}$ for every $\pi \in S_3$, i.e., $((x_1, x_2), (y_1, y_2)) \in R_{kl}$ iff $(\pi(x_1, x_2), \pi(y_1, y_2)) \in R_{kl}$.

Moreover, since any product of two orbits $P_{k_1k_2}$ and $P_{l_1l_2}$ is invariant under symmetric group S_3, the set of orbits (consequently the set of relations $R_{k_1k_2}$) is closed under multiplication. Also, if we use the notation $i=(i_1,i_2), j=(j_1,j_2)$ and $k=(k_1,k_2)$, it can be easily shown that, for $((x,x'),(y,y'))\in R_{k_1k_2}$, the intersection number

$$p_{ij}^k = |\{(z,z') : ((x,x'),(z,z'))\in R_{i_1i_2},\ \ ((z,z'),(y,y'))\in R_{j_1j_2}\}|$$

$$= |\{(z,z') : (z-x, z'-x')\in P_{i_1i_2},\ \ (y-z, y'-z')\in P_{j_1j_2}\}|, \tag{4-21}$$

is independent of the choice of $((x,x'),(y,y'))\in R_{k_1k_2}$. Therefore, the relations R_{kl} define an abelian association scheme (not necessarily symmetric) on $Z_m\times Z_m$, where in the regular representation of the group, for the corresponding adjacency matrices we have

$$A_{k,l}=\sum_{g\in P_{k,l}} g. \tag{4-22}$$

From (4-20) and (4-22), it follows that the adjacency matrices satisfy the following recursion relations

$$A_{10}A_{k,l} = A_{k+1,l}+A_{k,l-1}+A_{k-1,l+1}\ \ ,$$

$$A_{01}A_{k,l} = A_{k-1,l}+A_{k,l+1}+A_{k+1,l-1}\ \ , \tag{4-23}$$

where, $A_{00}=I$, A_{10} and $A_{01}=A_{10}^t$ are the first adjacency matrices. In fact, the following two matrices

$$A_z := S_1+S_2+(S_1S_2)^{-1}\ \ \text{and}\ \ A_{\bar{z}} := (A_z)^t, \tag{4-24}$$

generate the whole Bose-Mesner algebra of above constructed association schemes. In particular, $A_{kl}=p_{kl}(A_z,A_{\bar{z}})$, where p_{kl} is a polynomial of degree $k+l$ with real coefficients. We will refer to these types of association schemes as two-variable P-polynomial association schemes.

We illustrate the construction of underlying graph in simplest case $m=3$ in the following

Example: case $m=3$

From (4-20), the orbits of Weyl group S_3 are obtained as

$$P_{00}=\{(0,0)\},\ \ P_{10}=O((1,0))=\{(1,0),(0,1),(m-1,m-1)\},$$

$$P_{01} := O((0,-1)) = \{(2,0),(0,2),(1,1)\}, \quad P_{11} := O((1,-1)) = \{(1,2),(2,1)\}. \qquad (4\text{-}25)$$

Now by using (4-17), one can obtain the relations $R_{k_1k_2}$, for $(k_1,k_2) \in \{(0,0),(1,0),(0,1),(1,1)\}$. Also, it can be verified that $\Gamma(P) = \{R_{k_1k_2}\}$ is an abelian association scheme. The basis of Bose-Mesner algebra and dual Bose-Mesner algebra are

$$A_{00} = I_9, \quad A_{10} = S_1 + S_2 + (S_1S_2)^2, \quad A_{01} = S_1^2 + S_2^2 + S_1S_2, \quad A_{11} = S_1S_2^2 + S_1^2S_2 \text{ and}$$

$$E^*_{00} = {E'_0}^*\otimes{E'_0}^*, \quad E^*_{10} = {E'_0}^*\otimes{E'_1}^*+{E'_1}^*\otimes{E'_0}^*+{E'_2}^*\otimes{E'_2}^*, \quad E^*_{01} = {E'_0}^*\otimes{E'_2}^*+{E'_2}^*\otimes{E'_0}^*+{E'_1}^*\otimes{E'_1}^*,$$

$${E_{11}}^* = {E'_1}^* \otimes {E'_2}^* + {E'_2}^* \otimes {E'_1}^*, \qquad (4\text{-}26)$$

respectively, where

$$(E'^*_i)_{yy} = \delta_{yi}, \quad i = 0,1,2. \qquad (4\text{-}27)$$

The adjacency matrices are written in terms of A_z and $A_{\bar{z}}$ as follows

$$A_{00} = I, \quad A_{10} = A_z, \quad A_{01} = A_{\bar{z}}, \quad A_{11} = \frac{1}{3}(A_zA_{\bar{z}} - 3). \qquad (4\text{-}28)$$

One can notice that, the set $\{S_1, S_2\}$ is a generating set for $Z_m \times Z_m$, i.e., the elements of the group in the regular representation are of the form $(k,l) \doteq S_1^kS_2^l$, for $k,l \in \{0,1,...,m-1\}$. If we represent S_j as $S_j \doteq e^{2\pi i x_j/m}$, $x_j \in \{0,1,...,m-1\}$, then we have $S_jS_k = e^{2\pi i(x_j+x_k)/m}$, so the multiplication in the generating set $\{S_i, i=1,2\}$ is equivalent to the addition in the set $\{x_i, i=1,2\}$. In the additive notation, A_z is written as

$$A_z = e^{2\pi i x_1/m} + e^{2\pi i x_2/m} + e^{-2\pi i(x_1+x_2)/m}, \qquad (4\text{-}29)$$

so, clearly $\{(x_1, x_2, x_3 = -(x_1+x_2)) \ : \ x_i \in Z_m\}$ is a finite sequence of triples such that in the limit of large m tends to the root lattice A_2.

4.1.1 finite hexagonal lattice

The underlying graphs of two-variable P-polynomial association schemes constructed in previous section are directed graphs since the relation R_{10} is non-symmetric. In this section, in

order to obtain undirected (symmetric) underlying graphs of two-variable P-polynomial association schemes, we symmetrize the above constructed graphs of previous section. To do so, we choose a suitable union of the orbits such that the new partition Q is symmetric in the sense that $Q_{kl} = Q_{kl}^{-1}$, for all (k,l). In another words, we construct a blueprint from partition P, by symmetrization. Such a symmetrization conserves the property of being association scheme, because the union of the orbits is still invariant under the action of symmetric group. In appendix A of [16], such a symmetrization method is used for group association schemes.

Therefore, we construct the new underlying graph of association scheme, by choosing the generating set Q_{10} as follows

$$Q_{10} = P_{10} \cup P_{01} = \{(1,0),(0,1),(1,1),(m-1,0),(0,m-1),(m-1,m-1)\}. \tag{4-30}$$

With this choice, the adjacency matrix of underlying graph is

$$A = A_z + A_{\bar{z}}, \tag{4-31}$$

where, A_z and $A_{\bar{z}}$ are defined in (4-24). Clearly, the new graph can be viewed as finite hexagonal lattice. In the following, we give the symmetric partition Q and corresponding adjacency matrices of underlying graph for $m = 3$.

Example: case $m = 3$

Using (4-25), the new partition Q is given as

$$Q_{00} = \{(0,0)\}, \quad Q_{10} = \{(1,0),(0,1),(1,1),(m-1,0),(0,m-1),(m-1,m-1)\},$$

$$Q_{11} = P_{1,1} = \{(1,2),(2,1)\}, \tag{4-32}$$

and for the adjacency matrices, we have

$$A_{00} = I, \quad A_{10} = S_1 + S_2 + (S_1S_2)^2 + (S_1)^2 + (S_2)^2 + S_1S_2, \quad A_{11} = S_1S_2^2 + S_1^2S_2. \tag{4-33}$$

Clearly the new constructed graphs are also underlying graphs of two-variable P-polynomial association schemes. For example in the case of $m = 3$ we can write

$$A_{00} = 1, \quad A_{10} = A_z + A_{\bar{z}}, \quad A_{11} = \frac{1}{3}(A_zA_{\bar{z}} - 3), \tag{4-34}$$

In section 6, we will investigate the behavior of CTQW on these undirected graphs via spectral method, so we need to know the spectrum of adjacency matrix A. The spectrum of A_z in (4-24) can be easily determined as

$$z_{ij}=\omega^i+\omega^j+\omega^{-(i+j)},\quad \omega=e^{2\pi i/m};\quad i,j\in\{0,1,...,m-1\}. \tag{4-35}$$

Then, from (4-35) and that the spectrum of $A_{\bar{z}}$ is complex conjugate of the spectrum of A_z, one can calculate the spectrum of A as follows

$$\lambda_{kl}=z_{kl}+z^*_{kl}=2(\cos(2\pi k/m)+\cos(2\pi l/m)+\cos(2\pi(k+l)/m)). \tag{4-36}$$

4.2 construction of association scheme from two copies of hexagonal lattice

We extend the group $Z_m\times Z_m$ by direct product with Z_2 and obtain $Z_2\times Z_m\times Z_m$ as a vertex set for underlying graph of association scheme that we want to construct. As regards the argument of section 2, we know that, finite honeycomb lattice is equivalent to two copies of finite hexagonal lattice (see Fig.2), therefore we define the adjacency matrix A corresponding to finite honeycomb lattice, such that A^2 gives us $A_{hexagonal}$, the adjacency matrix of finite hexagonal lattice. That is we have

$$A=\sigma_+\otimes B^t+\sigma_-\otimes B, \tag{4-37}$$

where, $B=I+S_1+S_2^{-1}$. Clearly $B^tB=BB^t=S_1+S_2+S_1S_2+S_1^{-1}+S_2^{-1}+(S_1S_2)^{-1}=A_{hexagonal}$.

By computing the powers of adjacency matrix A, one can construct other adjacency matrices associated with an association scheme (not necessarily P-polynomial). Unfortunately, in this case we are not able to construct the association scheme via a systematic procedure based on group theoretical approach as in the case of finite hexagonal lattice (this shows the

preference of group theoretical approach). Also, it should be noted that, in this case the association scheme is defined in terms of matrices (see third definition of an association scheme in [9]). For example we give the adjacency matrices of Bose-Mesner algebra for $m = 3$.

case $m = 3$

The adjacency matrices of Bose-Mesner algebra are written as

$$A_0 = I_2 \otimes I_9, \quad A_1 = \sigma_+ \otimes B^t + \sigma_- \otimes B, \quad A_2 = I_2 \otimes A_{tri.},$$

$$A_3 = \sigma_+ \otimes (S_1 + S_2^2 + S_1S_2 + (S_1S_2)^2 + S_1^2S_2 + S_1S_2^2) + \sigma_- \otimes (S_1^2 + S_2 + (S_1S_2)^2 + S_1S_2 + S_1^2S_2 + S_1S_2^2),$$

$$A_4 = I_2 \otimes (S_1S_2^2 + S_1^2S_2). \quad (4\text{-}38)$$

One can see that A_i for $i = 1, ..., 4$ are symmetric and $\sum_{i=0}^{4} A_i = J_{18}$. Also it can be verified that, $\{A_i, \quad i = 1, ..., 4\}$ is closed under multiplication and therefore, the set of matrices $A_0, ..., A_4$ form a symmetric association scheme. We give only the following multiplications of adjacency matrices, where we will use them later

$$A_1^2 = 3A_0 + A_2, \quad A_1A_2 = 2A_1 + 2A_3, \quad A_1A_3 = 2A_2 + 3A_4, \quad A_1A_4 = A_3. \quad (4\text{-}39)$$

We will denote the graph constructed as above by Γ_s. It is notable that, in the limit of large m, the graph Γ_s can be viewed as a graph with vertices belonging to honeycomb lattice. In fact, starting from site e of a hexagonal lattice, the generators cI, cS_1^{-1} and cS_2 ($c^2 = 1$), generate the honeycomb lattice (See Fig.2). From Fig.2 one can see that, moving on the honeycomb lattice by steps of length two, is equivalent to moving on hexagonal lattice by steps of length one.

One can notice that, the graph Γ_s is a bipartite graph and has supersymmetric structure in the sense of Ref.[30], where we discuss the supersymmetric structure of Γ_s in appendix.

4.3 Stratification

In this section, first we recall some of the main features of stratification for underlying graphs of association schemes (see for example [16]) and then stratify the underlying graphs of association schemes constructed in previous subsections.

Let V be the vertex set of an underlying graph Γ of association scheme. For a given vertex $\alpha \in V$, the set of vertices having relation R_i with α is denoted by $\Gamma_i(\alpha) = \{\beta \in V : (\alpha, \beta) \in R_i\}$. Therefore, the vertex set V can be written as disjoint union of $\Gamma_i(\alpha)$ for $i = 0, 1, 2, ..., d$ (where, d is diameter of the corresponding association scheme), i.e.,

$$V = \bigcup_{i=0}^{d} \Gamma_i(\alpha). \tag{4-40}$$

Now, we fix a point $o \in V$ as an origin of the underlying graph, called reference vertex. Then, the relation (4-40) stratifies the graph into a disjoint union of strata (associate classes) $\Gamma_i(o)$.

With each stratum $\Gamma_i(o)$ we associate a unit vector $|\phi_i\rangle$ in $l^2(V)$ (called unit vector of i-th stratum) defined by

$$|\phi_i\rangle = \frac{1}{\sqrt{a_i}} \sum_{\alpha \in \Gamma_i(o)} |\alpha\rangle \in E_i^* W, \tag{4-41}$$

where, $|\alpha\rangle$ denotes the eigenket of α-th vertex at the associate class $\Gamma_i(o)$ and $a_i = |\Gamma_i(o)|$. For $0 \le i \le d$ the unit vectors $|\phi_i\rangle$ of Eq.(4-41) form a basis for irreducible submodule of corresponding Terwilliger algebra with maximal dimension denoted by W_0 ([11], Lemma 3.6). The closed subspace of $l^2(V)$ spanned by $\{|\phi_i\rangle\}$ is denoted by $\Lambda(G)$. Since $\{|\phi_i\rangle\}$ becomes a complete orthonormal basis of $\Lambda(G)$, we often write

$$\Lambda(G) = \sum_i \oplus \mathbf{C} |\phi_i\rangle. \tag{4-42}$$

In the graphs constructed from $Z_m \times Z_m$, the vertex set is $V = \{(k,l) : k, l \in \{0, 1, ..., m-1\}\}$. Therefore, for a given vertex $(m,n) \in V$, $\Gamma_{kl}((m,n)) = \{(m',n') : ((m,n),(m',n')) \in R_{kl}\}$ is equivalent to

$$\Gamma_{kl}((m,n)) = \{(m',n') : (m'-m, n'-n) \in O((k,-l))\}, \tag{4-43}$$

where, $O((k,-l))$ denote the orbits of Weyl group corresponding to the finite lattice. Now, we fix the vertex $(0,0) \in V$ as an origin of the underlying graph, called reference vertex. Then, the relation (4-40) stratifies the graph into a disjoint union of associate classes $\Gamma_{kl}((0,0))$. Then, the unit vectors (4-41) are written as

$$|\phi_{kl}\rangle = \frac{1}{\sqrt{a_{kl}}} \sum_{(m,n)\in\Gamma_{kl}((0,0))} |m,n\rangle, \tag{4-44}$$

where, $a_{kl} = |\Gamma_{kl}((0,0))|$. In section 6, we will deal with the CTQW on the constructed underlying graphs, where the strata $\{|\phi_{kl}\rangle\}$ span a closed subspace (irreducible submodule of corresponding Terwilliger algebra with maximal dimension called walk space), where the quantum walk remains on it forever.

For reference state $|\phi_{00}\rangle = |00\rangle$ we have

$$A_{kl}|\phi_{00}\rangle = \sum_{(m,n)\in\Gamma_{kl}((0,0))} |m,n\rangle. \tag{4-45}$$

Then by using unit vectors (4-44) and (4-45) one can see that

$$A_{kl}|\phi_{00}\rangle = \sqrt{a_{kl}}|\phi_{kl}\rangle. \tag{4-46}$$

In the case of finite honeycomb lattice, we have two sets of odd and even vertices, i.e., $V = V_o + V_e$, where V_o is the set of odd vertices defined by $V_o = \{(1;k,l) : k,l \in \{0,1,...,m-1\}\}$ and V_e is the set of even vertices defined by $V_e = \{(0;k,l) : k,l \in \{0,1,...,m-1\}\}$. We define stratum $\Gamma_i(u;k,l)$ as

$$\Gamma_i(u;k,l) = \{(v,k',l') : (A_i)_{((u;k,l),(v;k',l'))=1}\}, \tag{4-47}$$

where, $u,v \in 0,1$ and $k,l,k',l' \in \{0,1,...,m-1\}$. Now, we fix the vertex $(0;0,0) \in V$ as an origin of the underlying graph. Then, the relation (4-40) stratifies the graph into a disjoint union of associate classes $\Gamma_i((0;0,0))$ and the relations (4-44), (4-45) and (4-46) are satisfied by replacing $\Gamma_i(0,0)$ with $\Gamma_i((0;0,0))$.

One should notice that, these types of stratifications are different from the one based on distance, i.e., it is possible that two strata with the same distance from starting site posses different probability amplitudes.

5 Spectral distribution

In this section we give a brief review of spectral distributions for operators. Although the spectrum of underlying graphs on which we study CTQW, is easily evaluated and so CTQW can be investigated without spectral distribution approach, but in the limit of large size of the finite graphs, the best approach for calculating expected values of adjacency matrices is spectral distribution one. As we will see later, based on spectral distribution, one can approximate the behavior of the CTQW on infinite graphs with finite ones via stationary phase approximation method. Also, the spectral distribution approach is the best method for studying central limit theorems for quantum walks on graphs, see for example [31], [32].

In [16] and [17], CTQW on underlying graphs of QD type is investigated via spectral distribution, where the spectral measures associated with the adjacency matrices are single variable. In the case of n-variable P-polynomial association schemes, spectral measures are n-variable functions. Therefore, in the following we generalize the discussions in [16] and [17] to the case of n-variable P-polynomial association schemes.

It is well known that, for every set of commuting operators $(A_{z_1},...,A_{z_n})$ and a reference state $|\phi_0\rangle$, it can be assigned a distribution measure μ as follows

$$\mu(z_1,...,z_n)=\langle\phi_0|E(z_1,...,z_n)|\phi_0\rangle, \tag{5-48}$$

where $E(z_1,...,z_n)=\sum_i |u_i^{(z_1,...,z_n)}\rangle\langle u_i^{(z_1,...,z_n)}|$ is the operator of projection onto the common eigenspace of A_{z_1},...,A_{z_n} corresponding to eigenvalues z_1,...,z_n, respectively. Then, for any n-variable polynomial $P(A_{z_1},...,A_{z_n})$ we have

$$P(A_{z_1},...,A_{z_n})=\int...\int P(z_1,...,z_n)E(z_1,...,z_n)dz_1...dz_n, \tag{5-49}$$

where for discrete spectrum the above integrals are replaced by summation. Using the relations (5-48) and (5-49), we have

$$\langle\phi_0|P(A_{z_1},...,A_{z_n})|\phi_0\rangle = \int ... \int P(z_1,...,z_n)\mu(z_1,...,z_n)dz_1...dz_n. \tag{5-50}$$

The existence of a spectral distribution satisfying (5-50) is a consequence of Hamburgers theorem, see e.g., Shohat and Tamarkin [[33], Theorem 1.2].

Actually the spectral analysis of operators is an important issue in quantum mechanics, operator theory and mathematical physics [34, 35]. As an example $\mu(dx) = |\psi(x)|^2 dx$ ($\mu(dp) = |\widetilde{\psi}(p)|^2 dp$) is a spectral distribution which is assigned to the position (momentum) operator $\hat{X}(\hat{P})$. Moreover, in general quasi-distributions are the assigned spectral distributions of two hermitian non-commuting operators with a prescribed ordering. For example the Wigner distribution in phase space is the assigned spectral distribution for two non-commuting operators $\hat{X}$ (shift operator) and $\hat{P}$ (momentum operator) with Wyle-ordering among them [36, 37].

5.1 construction of orthogonal polynomials

As regards the arguments of section 4, the Bose-Mesner algebra corresponding to two-variable P-polynomial association scheme derived from orbits of Wyel group corresponding to finite hexagonal lattice, is generated by A_z and $A_{\bar{z}}$ defined by (4-24). We assign the variables z and $\bar{z}$ to A_z and $A_{\bar{z}}$, respectively. Then, in the limit of the large size of the underlying graph, the recursion relations (4-23) define a set of two-variable polynomials $p_{k,l}$ with the first polynomials and recursion relations as follows

$$P_{0,0} = 1, \quad P_{1,0} = z, \quad P_{0,1} = \bar{z} \ ,$$

$$zP_{k,l} = P_{k+1,l} + P_{k,l-1} + P_{k-1,l+1} \ ,$$

$$\bar{z}P_{k,l} = P_{k,l+1} + P_{k-1,l} + P_{k+1,l-1} \ , \tag{5-51}$$

where, the polynomials $P_{m,n}$ in (5-51) are orthogonal with respect to the constant measure $\mu(x_1, x_2) = 1$ (where, $z = e^{ix_1} + e^{ix_2} + e^{-i(x_1+x_2)}$), i.e., we have

$$\int_0^{2\pi}\int_0^{2\pi} P_{m,n}P_{m',n'}dx_1dx_2 = \delta_{m,m'}\delta_{n,n'}. \tag{5-52}$$

From (4-23) and (4-46), it can be seen that, there is a canonical isomorphism from the interacting Fock space of CTQW (irreducible submodule of Terwilliger algebra with highest dimension) on the symmetric underlying graphs of two-variable P-polynomial association schemes derived from $Z_m \times Z_m$ (finite hexagonal lattice) onto the closed linear span of the orthogonal polynomials generated by recursion relations (5-51). In fact, the adjacency matrices of non-symmetric association schemes constructed from $Z_m \times Z_m$ in section 4, are equal to polynomials $P_{m,n}(A_z, A_{\bar{z}})$ and the symmetrization of the association schemes is equivalent to realification of two-variable polynomials $P_{m,n}(z, \bar{z})$. Therefore, the adjacency matrices of symmetric association schemes derived from $Z_m \times Z_m$, are of the form $P_{m,n}(z, \bar{z})$ if $P_{m,n}(z, \bar{z})$ is real or of the form $P_{m,n}(z, \bar{z}) + \bar{P}_{m,n}(z, \bar{z})$ if $P_{m,n}(z, \bar{z})$ is complex.

It should be noted that, in the case of finite hexagonal lattice, the polynomials $P_{k,l}$ are not independent. Also, it can be shown that, these polynomials can be derived by using the raising operators A^+_z and $A^+_{\bar{z}}$ defined by (3-15) corresponding to symmetric underlying graphs. In the following, we list the strata and corresponding polynomials in the order of their first appearances as

$$|\phi_0\rangle \longrightarrow P_{0,0}$$

$$|\phi_{1,0}\rangle = A^+_z|\phi_0\rangle \rightarrow P_{1,0}, \quad |\phi_{0,1}\rangle = A^+_{\bar{z}}|\phi_0\rangle \rightarrow P_{0,1},$$

$$|\phi_{2,0}\rangle = (A^+_z)^2|\phi_0\rangle \rightarrow P_{2,0}, \;\; |\phi_{1,1}\rangle = A^+_z A^+_{\bar{z}}|\phi_0\rangle \rightarrow P_{1,1}, \;\; |\phi_{0,2}\rangle = (A^+_{\bar{z}})^2|\phi_0\rangle \rightarrow P_{0,2},$$

$$|\phi_{3,0}\rangle = (A^+_z)^3|\phi_0\rangle \rightarrow P_{3,0}, |\phi_{2,1}\rangle = (A^+_z)^2 A^+_{\bar{z}}|\phi_0\rangle \rightarrow P_{2,1}, |\phi_{1,2}\rangle = (A^+_{\bar{z}})^2 A^+_z|\phi_0\rangle \rightarrow P_{1,2}, |\phi_{0,3}\rangle = (A^+_{\bar{z}})^3|\phi_0\rangle \rightarrow$$

$$\ldots \tag{5-53}$$

For the sake of clarity, we construct the polynomials in the simplest case $m = 3$.

Example: case $m = 3$

In this case, we have $A^+_z=\sum_{i=0}^{2}{E''}^*_{i+1}A_z{E''}^*_i$ and $A^+_{\bar{z}}=\sum_{i=0}^{2}{E''}^*_{i+1}A_{\bar{z}}{E''}^*_i$, where A_z and $A_{\bar{z}}$ are given by (4-24) and the basis of dual Bose-Mesner algebra is given by

$$E''^*_0=E^*_0,\quad E''^*_1=E^*_1+E^*_2,\quad E''^*_2=E^*_3, \tag{5-54}$$

where, E^*_i for $i=0,1,2,3$ are given in (4-26). Now, by using A^+_z and $A^+_{\bar{z}}$, we obtain the following states

$$|\phi_{1,0}\rangle=A^+_z|00\rangle=|02\rangle+|20\rangle+|11\rangle=A_z|00\rangle,$$

$$|\phi_{0,1}\rangle=A^+_{\bar{z}}|00\rangle=|01\rangle+|10\rangle+|22\rangle=A_{\bar{z}}|00\rangle,$$

$$|\phi_{1,1}\rangle=A^+_zA^+_{\bar{z}}|00\rangle=3(|12\rangle+|21\rangle)=(A_zA_{\bar{z}}-3I)|00\rangle. \tag{5-55}$$

Therefore, the two-variable orthogonal polynomials associated with $|\phi_{1,0}\rangle$, $|\phi_{0,1}\rangle$ and $|\phi_{1,1}\rangle$ are

$$P_{1,0}=z,\quad P_{0,1}=\bar{z}\ \text{ and }\ P_{1,1}=z\bar{z}-3, \tag{5-56}$$

respectively. Moreover, the polynomials $P_{m,n}$ are special cases of orthogonal polynomials known as *generalized* Gegenbauer polynomials [25], [26]. These polynomials also can be derived from solving the schrodinger equation for special case of completely integrable quantum Calogero-Sutherland model of A_n type with constant potential, which describes the mutual interaction of $N=n+1$ particles moving on the circle. The coordinates of these particles are x_j, $j=1,...,N$ and the Schrodinger equation reads as

$$H\Psi=E\Psi,\quad H=-\frac{1}{2}\Delta,\qquad \Delta=\sum_{j=1}^{N}\frac{\partial^2}{\partial {x_j}^2}. \tag{5-57}$$

The ground-state energy and (non-normalized) wavefunction are

$$E_0=0,\quad \Psi_0(x_i)=1. \tag{5-58}$$

The excited states depend on an n-tuple of quantum numbers $m=(m_1,m_2,...,m_n)$:

$$H\Psi_m(x_i)=E_m\Psi_m,,\quad E_m=2(\lambda,\lambda), \tag{5-59}$$

where λ is the highest weight of the representation of A_n labeled by m, i.e., $\lambda = \sum_{i=1}^{n} m_i e_i$ and e_i are the fundamental weights of A_n. In fact, the eigenfunctions Ψ_m are solutions to the Laplace equation

$$-\Delta\Psi_m = E_m\Psi_m. \tag{5-60}$$

Let us restrict ourselves to the case A_2. If we change the variables as

$$z_1 = e^{2ix_1} + e^{2ix_2} + e^{2ix_3}, \quad z_2 = e^{2i(x_1+x_2)} + e^{2i(x_2+x_3)} + e^{2i(x_3+x_1)}, \quad z_3 = e^{2i(x_1+x_2+x_3)}, \tag{5-61}$$

then, in the center-of-mass frame ($\sum_i x_i = 0$), the wavefunctions depend only on two variables chosen as $z = z_1$ and $\bar{z} = z_2$ (in this case, $z_3 = 1$). With this change of variables and using normalization for Ψ_m such that the coefficient at the highest monomial is equal to one, we obtain the orthogonal polynomials P_{m_1,m_2} with respect to the constant measure Ψ_0 (the polynomials are correspond to exited states) which satisfy the recursion relations (5-51).

6 CTQW on underlying graphs of two-variable P-polynomial association schemes via spectral method

CTQW was introduced by Farhi and Gutmann in Ref.[5]. Let $l^2(V)$ denote the Hilbert space of C-valued square-summable functions on V (i.e., $\sum_i |f_i|^2 < \infty$). With each $\alpha \in V$ we associate a ket $|\alpha\rangle$, then $\{|\alpha\rangle, \ \ \alpha \in V\}$ becomes a complete orthonormal basis of $l^2(V)$.

Let $|\phi(t)\rangle$ be a time-dependent amplitude of the quantum process on graph Γ. The wave evolution of the quantum walk is

$$i\hbar\frac{d}{dt}|\phi(t)\rangle = H|\phi(t)\rangle, \tag{6-62}$$

where assuming $\hbar = 1$, and $|\phi_0\rangle$ be the initial amplitude wave function of the particle, the solution is given by $|\phi_0(t)\rangle = e^{-iHt}|\phi_0\rangle$. It is more natural to deal with the Laplacian of the graph defined by $L = A - D$ as hamiltonian, where D is a diagonal matrix with entries

$D_{jj} = \deg(\alpha_j)$ (recall that $\deg(\alpha_j)$ is degree of the vertex α_j defined by the number of edges incident to the vertex α_j). This is because we can view L as the generator matrix that describes an exponential distribution of waiting times at each vertex. But on d-regular graphs, $D = \frac{1}{d}I$, and since A and D commute, we get

$$e^{-itH} = e^{-it(A-\frac{1}{d}I)} = e^{-it/d}e^{-itA}, \qquad (6\text{-}63)$$

this introduces an irrelevant phase factor in the wave evolution. In this paper we consider $L = A = A_1$. Therefore, we have

$$|\phi_0(t)\rangle = e^{-iAt}|\phi_0\rangle. \qquad (6\text{-}64)$$

One approach for investigation of CTQW on graphs is using the spectral distribution method. CTQW on underlying graphs of P-polynomial association schemes has been discussed exhaustively in [15] via spectral method. In the following we investigate CTQW on underlying graphs of two-variable P-polynomial association schemes constructed in section 4 using spectral distribution method.

6.1 CTQW on underlying graphs of two-variable P-polynomial association schemes derived from $Z_m \times Z_m$

In the graphs constructed from $Z_m \times Z_m$, the adjacency matrix is written as $A_z + A_{\bar{z}}$ and so we assign polynomial $z + \bar{z}$ to adjacency matrix. Then, by using the relation (5-50), the expectation value of powers of adjacency matrix A over starting site $|\phi_{00}\rangle$ can be written as

$$\langle\phi_{00}|A^m|\phi_{00}\rangle = \int\int (z+\bar{z})^m \mu(z,\bar{z})dzd\bar{z}, \qquad m = 0,1,2,.... \qquad (6\text{-}65)$$

In the case of underlying graphs of two-variable P-polynomial association schemes, the adjacency matrices are two-variable polynomial functions of A_z and $A_{\bar{z}}$, hence using (4-46) and (6-65), the matrix elements $\langle\phi_{kl}|A^m \mid \phi_{00}\rangle$ can be written as

$$\langle\phi_{kl}|A^m \mid \phi_{00}\rangle = \frac{1}{\sqrt{a_{kl}}}\langle\phi_{00}|A_{kl}A^m \mid \phi_{00}\rangle = \frac{1}{\sqrt{a_{kl}}}\langle\phi_{00}|P_{kl}(A_z, A_{\bar{z}})A^m \mid \phi_{00}\rangle$$

$$= \frac{1}{\sqrt{a_{kl}}} \int_R \int_R (z+\bar{z})^m P_{kl}(z,\bar{z})\mu(z,\bar{z})dzd\bar{z}, \qquad m = 0,1,2,.... \tag{6-66}$$

One of our goals in this paper is the evaluation of amplitudes for CTQW on underlying graphs of two-variable P-polynomial association schemes constructed in section 4 via spectral distribution method. By using (6-66) we have

$$P_{kl}(t) = \langle\phi_{kl}|e^{-iAt}|\phi_{00}\rangle = \langle\phi_{kl}|\phi_{00}(t)\rangle = \frac{1}{\sqrt{a_{kl}}} \int_R \int_R e^{-i(z+\bar{z})t} P_{kl}(z,\bar{z})\mu(z,\bar{z})dzd\bar{z}, \tag{6-67}$$

where $\langle\phi_{kl}|\phi_{00}(t)\rangle$ is the amplitude of observing the particle at level kl (stratum $\Gamma_{kl}((0,0))$) at time t. One should notice that, as illustrated in section 5, the polynomials $p_{kl}(z,\bar{z})$ are obtained from realification of *generalized* Gegenbauer polynomials $P_{m,n}$ defined by (5-51). The conservation of probability $\sum_{k=0} |\langle\phi_{kl}|\phi_{00}(t)\rangle|^2 = 1$ follows immediately from (6-67) by using the completeness relation of orthogonal polynomials $P_{mn}(z,\bar{z})$. Obviously evaluation of $\langle\phi_{kl}|\phi_{00}(t)\rangle$ leads to the determination of the amplitudes at sites belonging to the stratum $\Gamma_{kl}((0,0))$.

Spectral distribution μ associated with the generators is defined as

$$\mu(z,\bar{z}) = \frac{1}{m^2}\sum_{k,l}\delta(z-z_{k,l})\delta(\bar{z}-z^*_{k,l}), \tag{6-68}$$

where $k,l \in \{0,1,...,m-1\}$. Now using (6-67) and spectral distribution (6-68), the probability amplitude of observing the walk at stratum $\Gamma_{ij}((0,0))$ at time t can be calculated as

$$P_{ij}(t) = \frac{1}{m^2}\sum_{k,l} e^{-2it(\cos 2\pi k/m+\cos 2\pi l/m+\cos 2\pi(k+l)/m)} p_{ij}(z_{k,l}, z^*_{k,l}). \tag{6-69}$$

In particular, the probability amplitude of observing the walk at starting site at time t is given by

$$P_{00}(t) := \frac{1}{m^2}\sum_{k,l} e^{-2it(\cos 2\pi k/m+\cos 2\pi l/m+\cos 2\pi(k+l)/m)}. \tag{6-70}$$

Example: case $m = 3$.

By using (4-35), we obtain $z_{kl} \in \{0,3,3\omega,3\omega^2\}$. Then by (6-68), spectral distribution is calculated as

$$\mu(z,\bar{z}) = \frac{1}{9}\{\delta(z-3)\delta(\bar{z}-3)+6\delta(z)\delta(\bar{z})+\delta(z-3\omega)\delta(\bar{z}-3\omega^2)+\delta(z-3\omega^2)\delta(\bar{z}-3\omega)\}. \tag{6-71}$$

Therefore, by using (4-34) and (6-67), probability amplitudes of observing the walk at starting site, stratum $\Gamma_{10}((0,0))$ and $\Gamma_{11}((0,0))$ are calculated as

$$P_{00}(t) = \frac{1}{9}\{e^{-6it} + e^{3it} + 6\},$$

$$P_{10}(t) = \frac{2}{3}\{e^{-6it} - e^{3it}\},$$

$$P_{11}(t) = \frac{2}{9}\{e^{-6it} + 2e^{3it} - 3\}, \tag{6-72}$$

respectively.

At the limit of the large m, we obtain the root lattice A_2 (hexagonal lattice). In the following we investigate the CTQW on root lattice A_2 using spectral method.

6.2 CTQW on hexagonal lattice

In this subsection we give continuous measure in the limit of the large size of the underlying graphs of symmetric two-variable P-polynomial association schemes derived by $A_z + A_{\bar{z}}$ in section 4.

In the limit of large m, the roots $z_{kl} = \omega^k + \omega^l + \omega^{-(k+l)}$ reduce to $z_{kl} = e^{ix_1} + e^{ix_2} + e^{-i(x_1+x_2)}$ with $x_1 = \lim_{k,m\to\infty} 2\pi k/m$ and $x_2 = \lim_{l,m\to\infty} 2\pi l/m$ and the spectral distribution given in (6-68), reduces to continuous constant measure $\mu(x_1, x_2) = 1/4\pi^2$.

Also, the measure μ can be given in terms of complex variables z and $\bar{z}$ as

$$\mu(z,\bar{z}) = \int_0^{2\pi}\int_0^{2\pi} dx_1 dx_2 \delta(z - (e^{ix_1} + e^{ix_2} + e^{-i(x_1+x_2)}))\delta(\bar{z} - (e^{-ix_1} + e^{-ix_2} + e^{i(x_1+x_2)})) =$$

$$= \frac{1}{4\pi^2\sqrt{-z^2\bar{z}^2 + 4(z^3 + \bar{z}^3) - 18z\bar{z} + 27}}. \tag{6-73}$$

Then, the probability amplitudes $P_{kl}(t)$ are given by

$$P_{kl}(t) = \langle\phi_{kl}|e^{-iAt}|\phi_{00}\rangle = \int_0^{2\pi}\int_0^{2\pi} dx_1 dx_2 e^{-2it(\cos x_1 + \cos x_2 + \cos(x_1+x_2))} p_{kl}(x_1, x_2), \tag{6-74}$$

where, $A_{kl} = p_{kl}(x_1, x_2)$. In particular, the probability amplitude of observing the walk at starting site at time t, is calculated as

$$P_{00}(t) = \int_0^{2\pi} \int_0^{2\pi} dx_1 dx_2 e^{-2it(\cos x_1 + \cos x_2 + \cos(x_1+x_2))}. \tag{6-75}$$

6.2.1 asymptotic behavior of quantum walk on hexagonal lattice

As regards argument of the end of section 4.1, we can not obtain an analytic expression for the amplitudes of the walk in the infinite case, i.e., the integral appearing in the (6-74) is difficult to evaluate, but we can approximate it for large time t by using the stationary phase method. Studying the large time behavior of quantum walk naturally leads us to consider the behavior of integrals of the form

$$I(t) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} dx_1 dx_2 g(\vec{x}) e^{-itf(\vec{x})} \tag{6-76}$$

as t tends to infinity. There is a well-developed theory of the asymptotic expansion of integrals which allows us to determine, very precisely, the leading terms in the expansion of the integral in terms of simple functions of t (such as inverse powers of t). Our basic technique will be to evaluate this integral in some approximation. The approximation we shall use will be the semiclassical expansion, which amounts to the well-known stationary phase approximation as applied to the path integral. In this approximation, one can evaluate $I(t)$ in (6-76) asymptotically as follows

$$\int \int dx_1 dx_2 g(\vec{x}) e^{-itf(\vec{x})} \simeq \sum_{\vec{a}} g(\vec{a}) e^{-itf(\vec{a})} \frac{2\pi}{it} (DetA)^{-1/2}, \tag{6-77}$$

where, summation is over all stationary points $\vec{a}$ of function $f(\vec{x})$ and A is Hessian matrix corresponding to $f(\vec{x})$. For more details about this approximation method, the reader is refered to [24].

Now, by using (6-77) we can discuss the asymptotic behavior of the amplitude of observing the quantum walk at starting site at large time t, i.e., we deal with the integral (6-76), with

$g(\vec{x}) = 1$ and

$$f(\vec{x}) = 2(\cos x_1 + \cos x_2 + \cos(x_1 + x_2)). \tag{6-78}$$

Therefore, for the asymptotic form of the amplitude $P_{00}(t)$ we get

$$I_0(t) \simeq \frac{\pi}{t}(\frac{1}{2\sqrt{3}}e^{-6it+i\pi/2} + \frac{1}{2}e^{2it} + \frac{1}{\sqrt{3}}e^{3it-i\pi/2}). \tag{6-79}$$

The asymptotic behavior of probability amplitudes $P_{kl}(t)$ ($kl \neq 00$) at large time t, can be evaluated similarly.

In order to obtain the asymptotic behavior of quantum walk on finite hexagonal lattice at large time t, we can compare the finite amplitude $P_{00}(t)$ (Eq.(6-70)) and the continuous probability (6-75) at large time t. Therefore, we calculate numerically the difference of amplitudes of the walk on root lattice A_2 with ones on finite hexagonal lattice, for large time t

$$\pi(m,t) = |I_0(t) - \frac{1}{m^2}\sum_{k,l=0}^{m-1} e^{-2it(\cos(\frac{2k\pi}{m})+\cos(\frac{2l\pi}{m})+\cos(\frac{2(k+l)\pi}{m}))}|. \tag{6-80}$$

The result has been depicted in Fig.3. The figure shows that, the difference $\pi(m,t)$ is limited to zero for m larger than ~ 50 and $t \sim 1000$. Therefore, to study the behavior of asymptotic quantum walk on finite hexagonal lattice, we can use arithmetic, approximate it with root lattice A_2, and by using the stationary phase method, study the behavior of asymptotic quantum walk.

6.3 CTQW on finite honeycomb lattice via spectral method

In the graph Γ_s constructed in section 4 from two copies of finite hexagonal lattices, we have

$$A = \sigma_+ \otimes B^t + \sigma_- \otimes B, \tag{6-81}$$

where, $B = I + S_1^{-1} + S_2$. Therefore, the spectrum of B is calculated as

$$z_{kl} = 1 + \omega^{-k} + \omega^l, \quad k,l \in \{0,1,...,m-1\}; \quad \omega = e^{\frac{2\pi i}{m}}, \tag{6-82}$$

and the eigenvalues of A are given by

$$\lambda_{kl} = \pm|z_{kl}| = \pm\sqrt{3 + 2(\cos(2\pi k/m) + \cos(2\pi l/m) + \cos(2\pi(k+l)/m))}. \qquad (6\text{-}83)$$

Now we apply spectral method by assigning variables z_1 and z_2 to B and B^t, respectively and a new variable z for σ_+ and σ_- commonly. Then, the variable assigned to adjacency matrix A will be $|z_1|z + |z_2|(z-1)$. Clearly we have $z_1 = z_2^*$ and so $|z_1| = |z_2|$. Therefore, we will have

$$A = |z_1|(2z-1). \qquad (6\text{-}84)$$

The spectral distribution associated with adjacency matrix A is given by

$$\mu(z_1, \bar{z_1}; z) = \frac{1}{2}\mu(z_1, \bar{z_1})(\delta(z) + \delta(z-1)), \qquad (6\text{-}85)$$

where,

$$\mu(z_1, \bar{z_1}) = \frac{1}{m^2}\sum_{k,l}\delta(z_1 - z_{kl})\delta(\bar{z_1} - z_{kl}^*). \qquad (6\text{-}86)$$

Then, the probability amplitude of observing the walk at stratum $\Gamma_k(0;00)$ at time t is calculated as follows

$$P_k(t) = \int\int\int e^{-i(|z_1|(2z-1))t}p_k(z_1;z)\mu(z_1, \bar{z_1}; z)dz_1 d\bar{z_1}dz; \quad k = 1,2,3,4, \qquad (6\text{-}87)$$

where, $A_k = p_k(z_1; z)$. In particular, the probability amplitude of observing the walk at starting site at time t is calculated as

$$P_0(t) = \int\int\int e^{-i(|z_1|(2z-1))t}\mu(z_1, \bar{z_1}; z)dz_1 d\bar{z_1}dz = \frac{1}{m^2}\sum_{k,l=0}^{m-1}\cos(\sqrt{3 + 2(cos 2\pi k/m + cos 2\pi l/m)})t. \qquad (6\text{-}88)$$

For the sake of clarity, in the following we give details for the case $m = 3$.

Example: case $m = 3$

From the relations (4-39), we have

$$A_0 = 1, \quad A_1 = p_1(z_1; z) = |z_1|(2z-1), \quad A_2 = p_2(z_1; z) = (|z_1|(2z-1))^2 - 3,$$

$$A_3 = p_3(z_1; z) = \frac{1}{2}|z_1|(2z-1)[(|z_1|(2z-1))^2-5], \quad A_4 = p_4(z_1; z) = \frac{1}{6}[(|z_1|(2z-1))^4+3(|z_1|(2z-1))^2]. \tag{6-89}$$

Using (6-82) and (6-83), the spectral distribution is obtained as

$$\mu(z_1, \bar{z_1}) = \frac{1}{9}\{\delta(z_1-3)\delta(\bar{z_1}-3)+2\delta(z_1-(2+\omega))\delta(\bar{z_1}-(2+\omega^2))+2\delta(z_1-(2+\omega^2))\delta(\bar{z_1}-(2+\omega))$$

$$+2\delta(z_1)\delta(\bar{z_1}) + \delta(z_1-(2\omega+1))\delta(\bar{z_1}-(2\omega^2+1)) + \delta(z_1-(2\omega^2+1))\delta(\bar{z_1}-(2\omega+1))\}. \tag{6-90}$$

Using (6-88), the probability amplitude of observing the walk at starting site at time t is calculated as

$$P_0(t) = \frac{1}{9}(\cos 3t + 6\cos\sqrt{3}t + 2). \tag{6-91}$$

Other probability amplitudes can be calculated using (6-87) and (6-89).

6.3.1 CTQW on honeycomb lattice

In the limit of the large m, the eigenvalues z_{kl} reduce to $z_{kl} = 1 + e^{-ix_1} + e^{ix_2}$ where $x_1 = \lim_{k,m\to\infty}\frac{2\pi k}{m}$ and $x_2 = \lim_{l,m\to\infty}\frac{2\pi l}{m}$. Therefore, the continuous spectral distribution is

$$\mu(z_1, \bar{z_1}) = \int_0^{2\pi}\int_0^{2\pi} dx_1 dx_2 \delta(z_1 - (1+e^{-ix_1}+e^{ix_2}))\delta(\bar{z_1} - (1+e^{ix_1}+e^{-ix_2})) =$$

$$\frac{1}{4\pi^2\sqrt{3 - z_1^2\bar{z_1}^2 - (z_1^2+\bar{z_1}^2) + 2z_1\bar{z_1}(z_1+\bar{z_1}) - 2(z_1+\bar{z_1})}}. \tag{6-92}$$

Therefore, in the limit of the large m, the probability amplitude of observing the walk at level k is given by

$$P_k(t) = \int_0^{2\pi}\int_0^{2\pi} dx_1 dx_2 (e^{i\sqrt{3+2(\cos x_1+\cos x_2+\cos(x_1+x_2))}t} p_k(x_1, x_2; 0) + e^{-i\sqrt{3+2(\cos x_1+\cos x_2+\cos(x_1+x_2))}t} p_k(x_1, x_2; 1 \tag{6-93}$$

In particular, for the probability amplitude $P_0(t)$ we have

$$P_0(t) = \int\int \cos(|z_1|t)\mu(z_1, \bar{z_1})dz_1 d\bar{z_1} = \int_0^{2\pi}\int_0^{2\pi} \cos\sqrt{3+2(\cos x_1+\cos x_2+\cos(x_1+x_2))}dx_1 dx_2 \tag{6-94}$$

6.3.2 asymptotic behavior

Similar to the finite hexagonal lattice, we investigate the asymptotic behavior of quantum walk at large time t using stationary phase approximation method. In this case we deal with the integral

$$I_0(t) = \int_0^{2\pi}\int_0^{2\pi} e^{-i(\sqrt{3+2(\cos x_1+\cos x_2+\cos(x_1+x_2))})t}dx_1dx_2+\int_0^{2\pi}\int_0^{2\pi} e^{+i(\sqrt{3+2(\cos x_1+\cos x_2+\cos(x_1+x_2))})t}dx_1dx_2, \tag{6-95}$$

as probability amplitude $P_0(t)$, so, by using the stationary phase method we approximate the integrals for large time t. Here, we have $g(x) = 1$ and $f(x_1, x_2) = \sqrt{3 + 2(\cos x_1 + \cos x_2 + \cos(x_1 + x_2))}$. Then the asymptotic form of the probability amplitude $P_0(t)$ is calculated as

$$I_0(t) \simeq \frac{\pi}{t}(2\sqrt{3}sin3t + 2cost). \tag{6-96}$$

Now, we compare the finite probability amplitude (6-88) and the continuous probability (6-96) at large time t. Therefore, we calculate numerically the difference between amplitude of walk on honeycomb lattice and finite one, for large time t

$$\pi(m,t) = |I_0(t) - \frac{1}{m^2}\sum_{k,l=0}^{m-1}\cos(\sqrt{3+2(\cos 2\pi k/m + cos 2\pi l/m)})t|. \tag{6-97}$$

The result has been depicted in Fig.4. The figure shows that, the difference $\pi(m,t)$ is limited to zero for $m \sim 60$ and $t \sim 700$. Therefore, to study the behavior of asymptotic quantum walk on finite honeycomb lattice, we can approximate it with infinite one, and by using the stationary phase method, study the behavior of asymptotic quantum walk.

7 Generalization to $Z_m^{\otimes n}$

Similar to the case $n = 2$, we choose generating set $P_{(10...0)} = \{(10...0), ..., (0...01), (m-1...m-1)\}$ for $Z_m^{\otimes n}$. Then, the orbits of Weyl group S_{n+1} which are indexed by n-tuple $m = (m_1, ..., m_n)$, are given by

$$P_m = O((m_1, -m_2, -m_2 - m_3, ..., -m_2 - m_3 - ... - m_n)). \tag{7-98}$$

By using (4-17) one can obtain a translation invariant partition R for $(Z_m^{\otimes n})^2$. In the regular representation, the adjacency matrix of underlying graph is written as

$$A_{z_1} = S_1 + ... + S_n + (S_1...S_n)^{-1}, \tag{7-99}$$

with $S_i = I \otimes ... \otimes \underbrace{S}_{i} \otimes I \otimes ... \otimes I$. Clearly, the relations R_m define an abelian association scheme (not necessarily symmetric) on $Z_m^{\otimes n}$. Moreover, the corresponding Bose-Mesner algebra is generated by

$$A_{z_k} = \sum_{i_1<i_2<...<i_k}^{n+1} S_{i_1}S_{i_2}...S_{i_k} \quad , \quad k = 1, ..., n, \tag{7-100}$$

where, $S_{n+1} = (S_1...S_n)^{-1}$. In the regular representation of the group, for the corresponding adjacency matrices we have

$$A_m = \sum_{g\in P_m} g \quad . \tag{7-101}$$

From (7-100) and (7-101), it follows that the adjacency matrices satisfy the following recursion relations

$$A_{z_k}A_m = \sum_{i_1<i_2<...<i_k}^{n+1} A_{m+v_{i_1}+...+v_{i_k}} \quad , \quad k = 1, ..., n, \tag{7-102}$$

where, v_i, for $i = 1, ..., n+1$, are n-dimensional vectors whose components are

$$(v_i)_l = \delta_{l,i} - \delta_{l,i-1} \quad , \quad l = 1, 2, ..., n. \tag{7-103}$$

In particular, $A_m = p_m(A_{z_1}, ..., A_{z_n})$, where p_m is a polynomial of degree $m_1 + ... + m_n$ with real coefficients. We refer to these types of association schemes as n-variable P-polynomial association schemes.

Now, we symmetrize the graph to obtain an undirected underlying graph as in the case of $n = 2$. Then, we will have for the adjacency matrix

$$A = A_{z_1} + A_{z_n}, \tag{7-104}$$

where, A_{z_1} is given by (7-99) and $A_{z_n} = (A_{z_1})^t$. The spectrum of A_{z_k} (indexed by n-tuple $l = (l_1, ..., l_n)$), is given by

$$z_l^{(k)} = \sum_{i_1<i_2<...<i_k}^{n+1} \omega^{l_{i_1}+...+l_{i_k}}, \quad l_i \in \{0, 1, ..., m-1\}, \tag{7-105}$$

where, $\omega = \exp^{2\pi i/m}$ and $l_{n+1} = -(l_1 + ... + l_n)$. From (7-105), on can see that the spectrum of A_{z_n} is complex conjugate of the spectrum of A_{z_1}. Therefore, the eigenvalues of A are given by

$$\lambda_{l_1,...,l_n} = 2(\cos 2\pi l_1/m + ... + \cos 2\pi l_n/m + \cos 2\pi(l_1 + ... + l_n)/m). \qquad (7\text{-}106)$$

The spectral distribution associated with the generators is given by

$$\mu(z_1, ..., z_n) = \frac{1}{m^n} \sum_{l_1,...,l_n} \delta(z_1 - z^{(1)}_{l_1..l_n})\delta(z_2 - z^{(2)}_{l_1..l_n})...\delta(z_n - z^{(n)}_{l_1..l_n}), \qquad (7\text{-}107)$$

where $l_i \in \{0, 1, ..., m-1\}$, for $i = 1, ..., n$. Now using (6-67) and spectral distribution (7-107), the amplitude of observing the walk at level $i = (i_1, ..., i_n)$ can be calculated as

$$P_i(t) = \frac{1}{m^n} \sum_{l_1,...,l_n} e^{-2it(\cos 2\pi l_1/m + ... + \cos 2\pi l_n/m + \cos 2\pi(l_1 + ... + l_n)/m)} p_i(z^{(1)}_{l_1..l_n}, ..., z^{(n)}_{l_1..l_n}), \qquad (7\text{-}108)$$

where, the polynomials $p_i(z_1, ..., z_n)$ are given by the following recursion relations

$$z_k P_m = \sum_{i_1<i_2<...<i_k}^{n+1} P_{m+v_{i_1}+...+v_{i_k}} \;, k = 1, ..., n, \qquad (7\text{-}109)$$

where, v_i for $i = 1, ..., n+1$ are defined by (7-103). In particular, the probability amplitude of observing the walk at starting site at time t is given by

$$P_0(t) := \frac{1}{m^n} \sum_{k,l} e^{-2it(\cos 2\pi l_1/m + ... + \cos 2\pi l_n/m + \cos 2\pi(l_1 + ... + l_n)/m)}. \qquad (7\text{-}110)$$

In the limit of large m, the eigenvalues $z_{l_1..l_n}$ reduce to $z_{l_1..l_n} = e^{ix_1} + ... + e^{ix_n} + e^{-i(x_1+...+x_n)}$ with $x_i = \lim_{l_i,m\to\infty} 2\pi l_i/m$, and the spectral distribution reduces to continuous constant measure $\mu(x_1, .., x_n) = 1/(2\pi)^n$. In fact, in the limit of large m, the study of CTQW on finite symmetric graph constructed from $Z_m^{\otimes n}$ as above, is equivalent to the study of walk on the root lattice A_n, where the continuous form of probability amplitude $P_i(t)$ is given by

$$P_i(t) = \frac{1}{(2\pi)^n} \int_0^{2\pi} ... \int_0^{2\pi} e^{-2it(\cos x_1 + ... + \cos x_n + \cos(x_1 + ... + x_n))} p_i(x_1, ..., x_n) dx_1...dx_n, \qquad (7\text{-}111)$$

where, $A_i = p_i(x_1, ..., x_n)$. In particular, the probability amplitude of observing the walk at starting site at time t is given by

$$P_0(t) = \frac{1}{(2\pi)^n} \int_0^{2\pi} ... \int_0^{2\pi} e^{-2it(\cos x_1 + ... + \cos x_n + \cos(x_1 + ... + x_n))} dx_1...dx_n, \qquad (7\text{-}112)$$

where, the integral in (7-112) can be approximated by employing stationary phase method at large time t.

8 conclusion

Using the spectral distribution method, we investigated CTQW on root lattice A_n and honeycomb one, by constructing two types of of association schemes and approximating the infinite lattices with finite underlying graphs of constructed association schemes, for large sizes of the graphs and large times. Although we focused specifically on root lattice A_n and honeycomb one, the underlying goal was to develop general ideas that might then be applied to other infinite lattices such as root lattices B_n, C_n and etc. also quasicrystals with certain symmetries. Apart from physical results, we succeeded to obtain some interesting mathematical results such as a generalization to the notion of P-polynomial association scheme, where we expect that, the n-variable P-polynomial association schemes posses the analogous properties of P-polynomial association scheme and can be applied in coding theory in order to construction of new codes. We hope that, studying other infinite lattices leads us to other interesting mathematical objects, perhaps new types of association schemes.

Appendix : Suppersymmetric structure of Γ_s

From the block form of A in (4-37), we can see that the constructed underlying graph of association scheme from two copies of finite hexagonal lattice, has supersymmetric structure. Following Ref.[30], we introduce the model of supersymmetric algebra as follows

We define two operators Q_+ and Q_- as

$$Q_+ = \begin{pmatrix} O & O \\ B & O \end{pmatrix}; \quad Q_- = \begin{pmatrix} O & B^t \\ O & O \end{pmatrix}. \tag{A-i}$$

Then we define two hermitean charges Q_1, Q_2 and Hamiltonian H as follows

$$Q_1 = Q_+ + Q_-, \quad Q_2 = -i(Q_+ - Q_-), \quad H = Q_1^2 = Q_2^2. \tag{A-ii}$$

With the above definitions, we get

$$Q_+^2 = Q_-^2 = 0, \quad H = \{Q_+, Q_-\}, \quad [H, Q_\pm] = 0, \quad [H, Q_{1,2}] = 0,$$

$$\{Q_1, Q_2\} = 0, \quad \Rightarrow \quad \{Q_i, Q_j\} = 2H\delta_{ij}. \tag{A-iii}$$

Therefore, Q_+, Q_- and H generate a closed supersymmetric algebra.

For the association scheme derived from two copies of finite hexagonal lattice in section 4, we make the following correspondence

$$Q_1 = A = \begin{pmatrix} O & B^t \\ B & O \end{pmatrix}, \quad Q_2 = \begin{pmatrix} O & iB^t \\ -iB & O \end{pmatrix}, \tag{A-iv}$$

and therefore,

$$H = A^2 = \begin{pmatrix} B^tB & O \\ O & BB^t \end{pmatrix}; \quad Q_+ = \begin{pmatrix} O & O \\ B & O \end{pmatrix}, \quad Q_- = \begin{pmatrix} O & B^t \\ O & O \end{pmatrix}. \tag{A-v}$$

In other words, the adjacency A is our original Dirac operator. Now it can be checked that all the above (anti) commutation relations are fulfilled by our representation in the form of graph operators. In our special graph, B and B^t commute with each other, so the Hamiltonian is of the form $H = I \otimes B^tB$. Therefore, the spectrum of H is at least twofold degenerate, i.e.,

$$H(f,g)^t = E(f,g)^t \quad \Rightarrow \quad B^tBf = Ef, \quad B^tBg = Eg. \tag{A-vi}$$

Hence, $(f,0)^t$ and $(0,g)^t$ are eigenvectors of H to the same eigenvalue.

As $H = Q_1^2 = Q_2^2$ and $\{Q_1, Q_2\} = 0$, certain combinations of the above eigenvectors yield common eigenvectors of the pairs H, Q_i.

From the fact that $[B, B^t] = 0$, we know that B and B^t have common eigenvectors. If

$$Bf = \lambda f, \quad B^tf = \lambda' f, \tag{A-vii}$$

then

$$BB^t f = \lambda\lambda^{'} f. \tag{A-viii}$$

As the spectrum of B is complex conjugate of the spectrum of B^t, we have

$$BB^t f = |\lambda|^2 f. \tag{A-ix}$$

In other words, the eigenvector of B with eigenvalue λ, is eigenvector of Hamiltonian H, with eigenvalue $|\lambda|^2$ and degeneracy at least 2.

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Figure Captions Figure-1: Shows root system corresponding to A_2.

Figure-2: Shows finite honeycomb lattice with generators cI, cS_1^{-1} and cS_2.

Figure-3: Shows $\pi(m,t)$ for root lattice A_2 as a function of m (where, m^2 is the number of vertices of finite hexagonal lattice) at $t \sim 1000$, where the difference is almost negligible for $m \geq 50$.

Figure-4: Shows $\pi(m,t)$ for honeycomb lattice as a function of m (where, $2m^2$ is the number of vertices of finite honeycomb lattice) at $t \sim 700$, where the difference is almost negligible for $n \geq 60$.

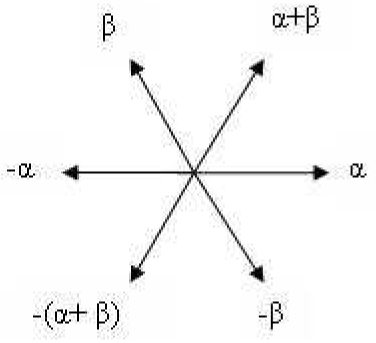


Fig.1

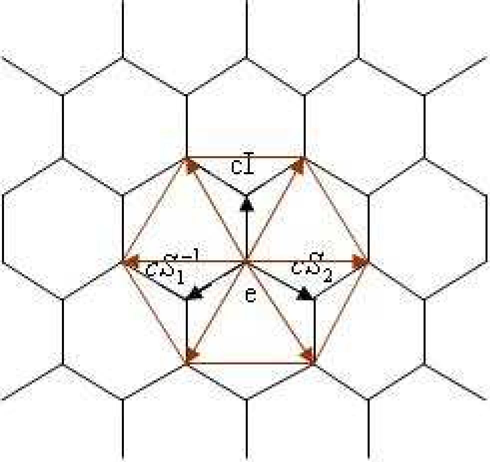
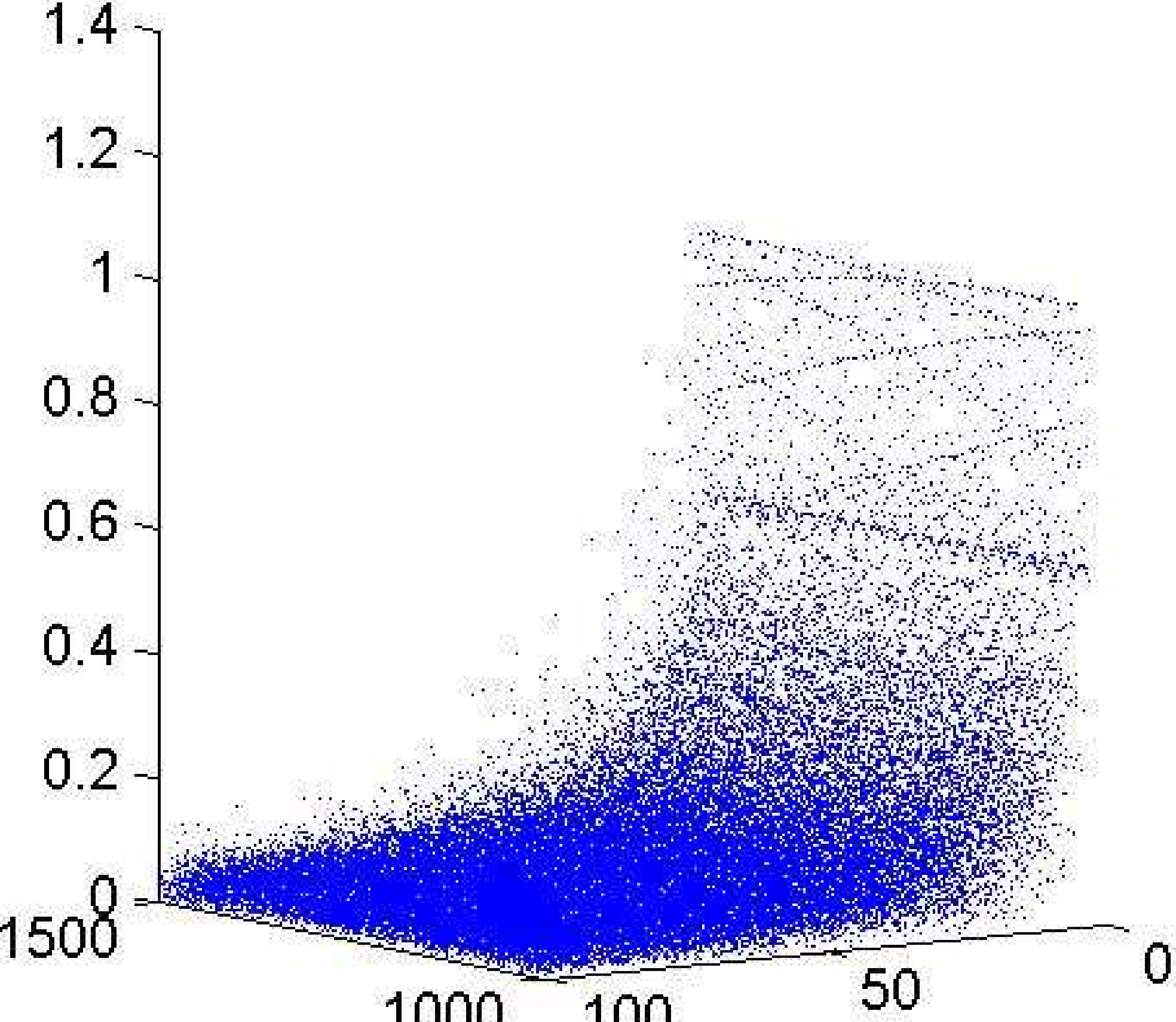


Fig.2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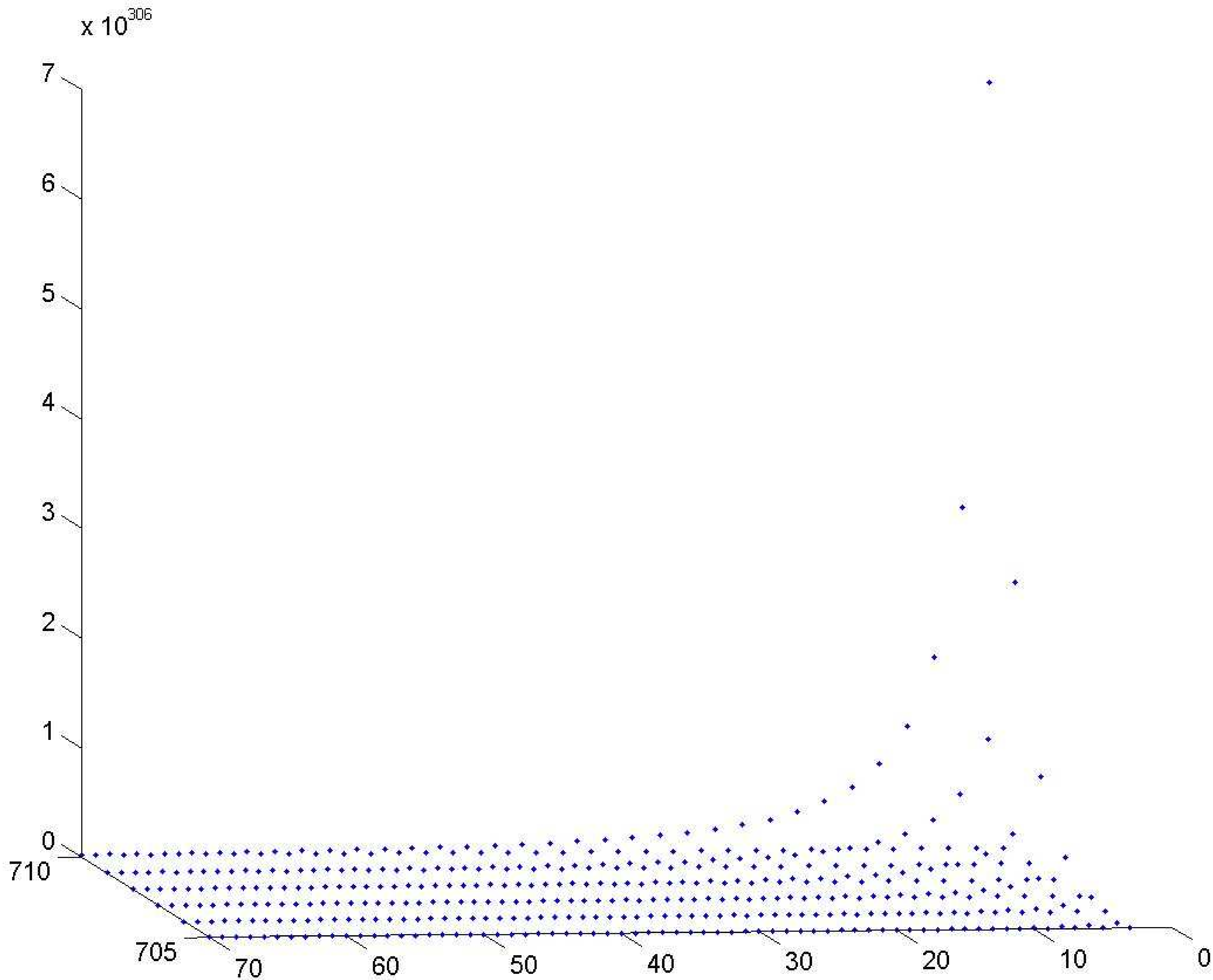
1.2
1
0.8
0.6
0.4
0.2
0
1500
1000
100
50
0



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7
6
5
4
3
2
1
0
710
705
70
60
50
40
30
20
10
0